

Mean first passage time for nuclear fission and the emission of light particles

Helmut Hofmann¹ and Fedor A. Ivanyuk^{1,2}

1) *Physik Department, TUM, D-85747 Garching, Germany*

2) *Institute for Nuclear Research, 03028 Kiev, Ukraine*

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The concept of a mean first passage time is used to study the time lapse over which a fissioning system may emit light particles. The influence of the "transient" and "saddle to scission times" on this emission are critically examined. It is argued that within the limits of Kramers' picture of fission no enhancement over that given by his rate formula need to be considered.

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Introduction — Fission at finite thermal excitation is characterized by the evaporation of light particles and γ 's. Any description of such a process must rely on statistical concepts, both with respect to fission itself as well as with respect to particle emission. For decades it has been customary to describe experiments in terms of particle [1] and fission widths, where the former, Γ_n , is identified through the evaporation rate and the latter Γ_f is given by the Bohr-Wheeler formula $\Gamma_f \equiv \Gamma_{BW}$ for the fission rate. Often in the literature this is referred to as the "statistical model". It was only in the 80's that discrepancies of this procedure with experimental evidence was encountered: Sizable more neutrons were seen to accompany fission events than given by the ratio Γ_n/Γ_{BW} (for a review see e.g. [2]). A possible enhancement of that ratio is found if the fission width Γ_{BW} is replaced by the Γ_K of Kramers [3]. In this seminal paper he pointed to the deficiency of the picture of Bohr and Wheeler in that it discards the influence of couplings of the fission mode to the nucleonic degrees of freedom. Such couplings will in general reduce the flux across the barrier, mainly because of the reduction of the energy in the fission degree of freedom Q which may then fall below the barrier. This Q is meant to represent the most likely path in a multidimensional landscape of shape degrees of freedom.

In Kramers' picture this effect is realized through the presence of frictional and fluctuating forces (intimately connected to each other by the fluctuation dissipation theorem). Presently it is understood that Kramers' "high viscosity limit" applies (for a microscopic justification see [4, 5]), in which case the rate formula writes

$$\Gamma_K = \frac{\hbar \omega_a}{2\pi} \exp\left(-\frac{E_b}{T}\right) \left(\sqrt{1 + \eta_b^2} - \eta_b\right) = \frac{\hbar}{\tau_K}. \quad (1)$$

Here, T and E_b stand for temperature and barrier height, ω_a for the frequency of the motion around the minimum at $Q = Q_a$ and $\eta_b = (\gamma/(2M\omega))_b$ for the dissipation strength at the barrier (at $Q = Q_b$) with γ being the friction coefficient and M the inertia. For the sake of simplicity we will assume these coefficients not to vary along the fission path; otherwise the formula must be modified [5]. For vanishing dissipation strength (1) reduces to the Bohr-Wheeler formula (simplified to the case that

the equilibrium of the nucleons can be parameterized by a temperature).

Commonly, formula (1) is derived (see e.g. [6]) in a time dependent picture solving the underlying Fokker-Planck equation for special initial conditions with respect to the time dependence of the distribution function [7]. Their choice is intimately related to the picture of a compound reaction, in that the decay process is assumed to be independent of how the compound nucleus is produced. The latter in a sense represents a nucleus in a quasi-equilibrium such that the previous, pre-equilibrium stages need not be considered explicitly. This assumption is valid as long as the decay of that system takes longer than the equilibration time. To some large extent such a situation is indeed given at not too high excitations, as then the nucleons may stay inside this nuclear complex for a sufficiently long time. However, the circumstances are less clear with respect to the collective modes, in particular to the fission degree of freedom itself — which for large damping probably is among the slowest ones present. Whereas the corresponding kinetic momentum $P = M\dot{Q}$ may safely be assumed to equilibrate sufficiently fast, this may not be so for the coordinate Q . Thus, assuming the system to be located initially around the supposedly pronounced "ground state" minimum of the static energy at $Q = Q_a$, the initial width in Q may still be at one's disposal. In its true spirit the compound picture would suggest taking the equilibrium value, determined by the temperature and, in harmonic approximation, by the stiffness of the potential. Often, however, one starts with a sharp distribution of zero width. In any case, the current across the barrier needs some finite time to build up. This apparent *delay* of fission was interpreted [8, 9] as if there was the *additional* possibility of emitting light particles *beyond* the measure given by $\Gamma_n/\Gamma_K > \Gamma_n/\Gamma_{BW}$.

If besides collective motion also particle emission is studied explicitly in a time dependent picture, as done in the Langevin approach [10, 11], such an effect is included automatically. Problems arise, however, if one tries to imitate this delay in statistical codes which are in use for analyzing experimental results. Such codes apply static probabilities derived in *time independent* reaction theory. It is not obvious how this method may be reconciled with the picture of fission delay, the "transient effect". In the

present note we like to shed some light on this problem by exploiting the concept of a mean first passage time (MFPT). Before we shall come to that we want to examine a little closer the time dependent case. We will concentrate on over-damped motion, as in this case the MFPT can be evaluated from an analytic formula. Moreover, for slow motion the transient time gets larger, such that the feature we want to discuss becomes even more obvious.

Time dependent current across the barrier — In the time dependent picture just described the boundary conditions in Q (and P if present) are chosen to make sure that the distribution vanishes at infinity. Calculations of the current $j(t)$ across the barrier then typically imply a behavior as exhibited in Fig.1. In all cases the asymptotic value of $j_b(t)$ is seen to follow the law $\Gamma_K \exp(-\Gamma_K t/\hbar)$, shown by the fully drawn straight line. The differences at short times are due to the following different initial conditions:

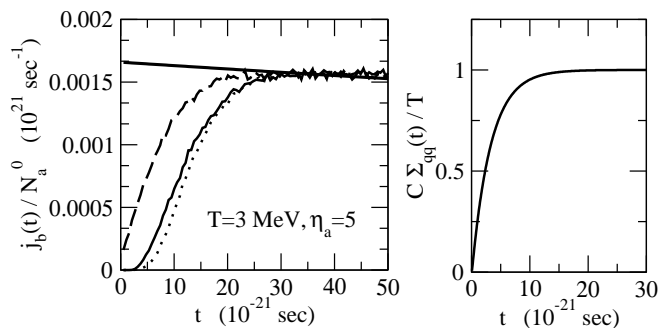


FIG. 1: The current across the barrier for different initial conditions, see text.

(i) For the dashed and dotted curves the system starts out of equilibrium in Q ; the dashed curve corresponds to the current at the barrier $j_b(t) = j(Q_b, t)$ and the dotted one to that in the scission region $j_{sc}(t) = j(Q_{sc}, t)$, beyond which the fragments separate. The equilibrium is defined by the oscillator potential by which the $V(Q)$ around Q_a may be approximated.

(ii) For the fully drawn line the system starts at Q_a sharp. The obvious delay by about $5 - 10 \cdot 10^{-21}$ sec is essentially due to the relaxation of Q to the quasi-equilibrium in the well. This feature is demonstrated on the right by the t -dependence of the width in Q (exhibited in terms of fluctuations of the potential energy $C\Sigma_{qq} = C(\langle Q^2 \rangle - \langle Q \rangle^2)/2$).

The figure clearly demonstrates remarkable uncertainties in the very concept of the "transient effect". First of all it is seen, that the "transient" time τ_{trans} , defined as the time the current $j_b(t)$ needs to reach its asymptotic behavior, depends strongly on the initial conditions. Moreover, there is considerable arbitrariness in choosing time zero: If the calculation were repeated at some later time $t_0 > \tau_{trans}$, the same features would be seen! In the end this is due to the very fact that the whole effect only comes about because in the initial distribution there are favorable parts for which it is easiest to reach the barrier.

This is demonstrated in Fig.2. There, those points of the initial equilibrium are sampled which cross the barrier after some given time τ_s . On the right a sufficiently large τ_s was chosen such that *greater parts* of the initial distribution have "fissioned". As exhibited on the left, for the much shorter time $\tau_s \simeq \tau_{trans}$, only a small fraction of points have succeeded in doing this, namely those which started close to the barrier (for under-damped motion also more favorite initial momenta would play a role, see [12, 13]). The vast majority of particles is still waiting to complete the same motion but at later times! This aspect is important, not only for an understanding of the essentials of the concept of the MFPT [14, 15, 16], but also in respect to the evaporation of neutrons. Indeed, even for $\tau_K \gtrsim t \gg \tau_{trans}$ there is ample time for them to be emitted from *inside* the barrier.

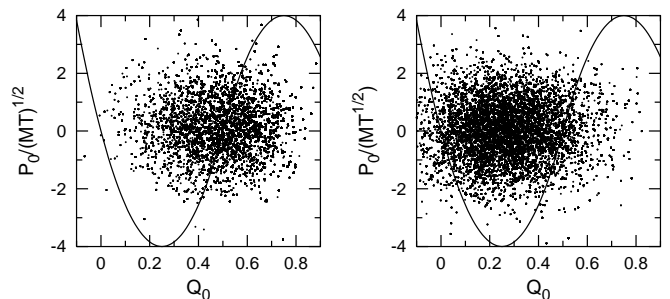


FIG. 2: Samples of initial points which overcome the saddle within a time τ_s : Left part: $\tau_s \simeq \tau_{trans}$; right part $\tau_s \simeq \tau_K$.

The calculations have been performed by simulating the Langevin equations exploiting a locally harmonic approximation similar to that of [4, 6] for Kramers' equation, for the following parameters: $T = 3$ MeV, $E_b = 8$ MeV, $\hbar\omega_a = 1$ MeV and $\eta_a = 5$. The potential was constructed from two oscillators, one upright and one upside down, joined with a smooth first derivative.

The mean first passage time — Within a Langevin approach the concept of MFPT may be described as follows. Suppose that at $t = 0$ particles start at the potential minimum Q_a . Because of the fluctuating force there will be trajectories i which pass a certain exit point Q_{ex} first at some time t_i , the *first passage time*. The *mean-FPT* $\tau_{mfpt}(Q_a \rightarrow Q_{ex})$ is defined by the average $\langle t_i \rangle$ over all possibilities. In order to really obtain the mean *first* passage time the i has to be removed from the ensemble once it has exited the interval at Q_{ex} : the "particle" can be said to be absorbed at Q_{ex} (such that one may speak of an "absorbing barrier"). As the potential $V(Q)$ is assumed to rise to infinity for $Q \rightarrow -\infty$, any motion to the far left will bounce back: the region $Q \rightarrow -\infty$ acts as a "reflecting barrier". A calculation of the MFPT with the Langevin equation is shown in Fig.3 by the dashed double dotted curve and seen to be very close to the result obtained by exploiting special solutions of the Smoluchowski equation, which we want to address now.

Fortunately, the Smoluchowski approach allows one to derive an analytic formula for the τ_{mfpt} [14, 15, 16]. As one knows, the Smoluchowski equation represents that

of Kramers for over-damped motion. For its solution $K(Q, t | Q_a, 0)$ the initial condition for the particles to start at Q_a is given by $\lim_{t \rightarrow 0} K(Q, t | Q_a, 0) = \delta(Q - Q_a)$, which is identical to the one used for the fully drawn line of Fig.1. For constant friction and temperature one gets

$$\tau_{\text{mfpt}} = \frac{\gamma}{T} \int_{Q_a}^{Q_{\text{ex}}} du \exp \left[\frac{V(u)}{T} \right] \int_{-\infty}^u dv \exp \left[-\frac{V(v)}{T} \right]. \quad (2)$$

This expression may be derived as follows: The probability of finding at time t the particle still inside the interval $(-\infty, Q_{\text{ex}})$ is given by $W(Q_a, t) = \int_{-\infty}^{Q_{\text{ex}}} dQ \times K(Q, t | Q_a, 0)$. Hence, the probability for it to leave the region during the time lapse from t to $t+dt$ is determined by $-dW = -(\partial W(Q_a, t)/\partial t) dt$, such that the average time becomes $\tau_{\text{mfpt}}(Q_a \rightarrow Q_{\text{ex}}) = -\int t dW$ which turns into

$$\begin{aligned} \tau_{\text{mfpt}}(Q_a \rightarrow Q_{\text{ex}}) &= \int_0^\infty \int_{-\infty}^{Q_{\text{ex}}} K(Q, t | Q_a, 0) dQ dt \\ &= \int_0^\infty dt t j(Q_{\text{ex}}, t | Q_a, 0). \end{aligned} \quad (3)$$

These formulas are associated to the special boundary conditions with respect to the coordinate mentioned be-

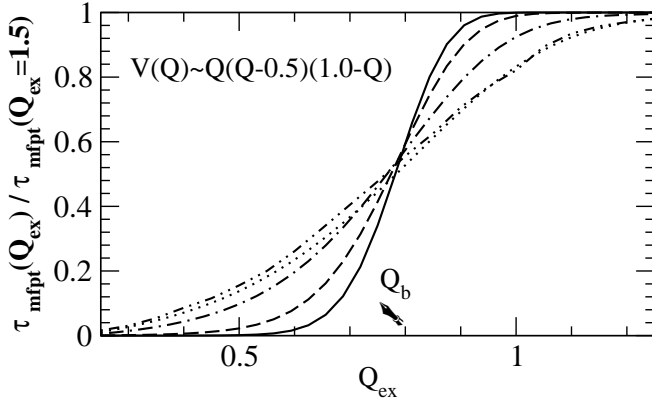


FIG. 3: MFPT for a cubic potential normalized to its asymptotic value, shown by the solid, dashed, dotted-dashed and dotted curves which correspond to $T/E_b = 0.1, 0.2, 0.5, 1.0$. The dashed double dotted curve represents a calculation within the Langevin approach for $T/E_b = 1$.

fore, the reflecting barrier at $Q \rightarrow -\infty$ and an absorbing barrier at Q_{ex} . In particular for the latter feature it is not permitted to use in (3) the currents shown in Fig.1. Inserting them blindly would indeed lead to expressions for τ_{mfpt} in which the τ_{trans} appears [17]. *This is in clear distinction to the correct form (2)*. Actually, the derivation of (2) involves proper solutions of that equation which is "adjoint" to the Smoluchowski equation, and which describes motion backward in time. In Fig.3 we show the dependence of $\tau_{\text{mfpt}}(Q_a \rightarrow Q_{\text{ex}})$ on Q_{ex} as given by (2) calculated for a cubic potential. Evidently, the MFPT needed to reach the saddle at Q_b is *exactly half the asymptotic value*. The latter may be identified as

the mean fission life time $\tau_f \equiv \tau_{\text{mfpt}}(Q_a \rightarrow Q_{\text{ex}} \gg Q_b)$. For the typical conditions under which Kramers' rate formula (1) is valid for overdamped motion, the identity of $\tau_f \equiv \tau_K$ to the asymptotic value of the MFPT can be proven analytically [15]. Another remarkable feature seen in Fig.3 is the insensitivity of the MFPT to the exit point for small and large Q_{ex} . Actually, in clear distinction to the transient time the MFPT is also insensitive to the starting point. This latter property shall be exhibited in a forthcoming paper [13].

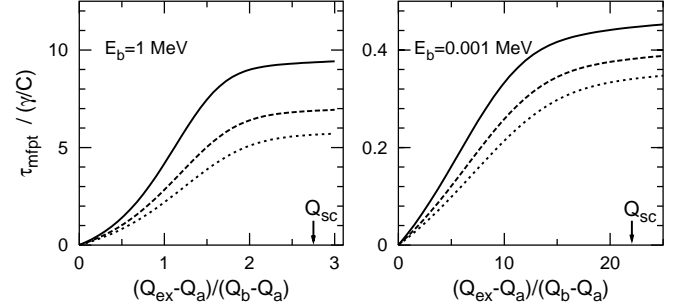


FIG. 4: The MFPT for the case of small and vanishing barriers for $T = 2, 3, 4$ MeV from top to bottom. The Q_{sc} corresponds to a scission point 20 MeV below the barrier.

As a most interesting feature, the MFPT can be calculated also for cases of small barriers where Kramers' formula does not apply. We show in Fig.4 results of evaluations of formula (2) for $E_b = 1$ MeV as well as for a practically vanishing barrier. It is seen that even in the latter case the $\tau_{\text{mfpt}}(Q_a \rightarrow Q_{\text{ex}})$ reaches a plateau for sufficiently large Q_{ex} . This asymptotic value, however, is no longer determined by τ_K . Nevertheless, the τ_{mfpt} seems to be long enough for neutrons to be evaporated before scission. This may be seen as follows. The neutron width typically is of the order of $1 \dots 3$ MeV (for medium heavy nuclei [10]). According to [5] the γ/C roughly increases linearly in T , being about $1 \hbar/\text{MeV}$ at $T = 2$ MeV and about $3 \hbar/\text{MeV}$ at $T = 3$ MeV. Taking the values of τ_{mfpt} from the right part of Fig.4 and close to the plateau one gets a width $\Gamma_{\text{mfpt}} = \hbar/\tau_{\text{mfpt}}$ of the order of $0.9 \dots 2.3$ MeV, and thus comparable to the neutron width. Fig.4 also shows that a small increase of the barrier by 1 MeV enlarges the τ_{mfpt} drastically. *Discussion* — It should be evident from the previous discussion that in the very concept of the MFPT there is no room for a transient effect. After all, formula (2) is based on *exact solutions of the transport equation which satisfy the same initial condition as those used for the plots in Fig.1* — albeit different boundary conditions in coordinate space. Moreover, as exhibited in Fig.2 the evaluation of the MFPT takes into account an average over *all* initial points, as is warranted by the definition of the MFPT through the probability distribution $-dW$. Contrasting this feature, and as outlined in the second section, the transient effect only represents a minor part of the initial population, namely that one which reaches the barrier first. Discarding the rest implies ignoring the many particles which are

still moving inside the barrier for times typically much longer than τ_{trans} . Hence, neutrons from deformations corresponding to that region may not only be emitted within τ_{trans} but within $\tau_{\text{mfpt}}(Q_a \rightarrow Q_b)$, which turns out to be just half of the total fission time τ_K . Of course, this discussion shows that it is also not correct to argue in favor of "additional" neutrons which might be emitted within the saddle to scission time τ_{ssc} introduced in [18]. As one may guess from Fig.3, like the τ_{trans} , the τ_{ssc} does not appear to be in accord with the MFPT either: The time the fissioning system stays together is not determined by motion in the immediate neighborhood of the barrier. On average it takes half the full decay time to move beyond the Q_b to the Q_{ex} at which the τ_{mfpt} reaches its plateau value.

These findings suggest that one simply estimates the emission rate of neutrons over fission from the ratio Γ_n/Γ_K — provided one may trust the potential to be of the simple form underlying the rate formula (1). Anything else does not seem to be in accord with an appropriate application of Kramers' or Smoluchowski's equations. This does not rule out other, complementary effects which originate in more complicated situations. For instance, in case that in the scission region the potential becomes flat again or even develops a minimum the system is forced to stay there longer than given by the τ_K of eq.(1) — implying additional time for evaporating neutrons. Likewise it is conceivable that the *initial* stage of the whole reaction is to be described with a *dif-*

ferent transport model. Such modifications are already suggested when the average neutron emission time τ_n becomes comparable to or even smaller than the relaxation time τ_{micro} for the nucleonic degrees of freedom as a whole. Transport equations are justified only if this τ_{micro} is the smallest time scale present, in comparison to both neutron emission as well as to collective motion. The τ_{micro} turns out to be of the order of $1 - 2 \cdot 10^{-22}$ sec, no matter whether it is estimated within linear response theory with collisional damping or within a random matrix approach (see [4]). Applying the Weisskopf estimate for the neutron emission time (or modified versions of it) [10] at large temperatures one easily gets values of τ_n of the order of or smaller than τ_{micro} . This reflects a situation of *pre-equilibrium* rather than that assumed in the quasi-static picture necessary for the application of Fokker-Planck equations. In conclusion we may say that deviations of experimental results from the standard value of Γ_n/Γ_K ought perhaps to be understood as a strong indication of the relevance of these complementary effects, which unfortunately have for the most part been unconsidered. This might require one to re-examine analyzes of experiments which over the past decade or so have followed the conventional line.

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